

# Interaction of vortices in thin superconducting films and Berezinskii-Kosterlitz-Thouless transition

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The precondition for the BKT transition in thin superconducting films, the logarithmic intervortex interaction, is satisfied at distances short relative to  $\Lambda = 2\lambda^2/d$ ,  $\lambda$  is the London penetration depth of the bulk material and  $d$  is the film thickness. For this reason, the search for the transition has been conducted in samples of the size  $L < \Lambda$ . It is argued below that film edges turn the interaction into near exponential (short-range) thus making the BKT transition impossible. If however the substrate is superconducting and separated from the film by an insulated layer, the logarithmic intervortex interaction is recovered and the BKT transition should be observable.

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*Introduction.* The seminal prediction by Berezinskii [1], Kosterlitz, and Thouless [2] (BKT) of the phase transition caused by fluctuations-induced topological excitations in two-dimensional (2D) systems has been confirmed in a number of experiments with superfluid films. Many attempts to do the same with thin superconducting films were less convincing, for a review of early theoretical and experimental work see, e.g., Ref. 3. Later transport data on superconducting films remained inconclusive [4, 5]. The recent transport measurements [6] on high quality ultra-thin high- $T_c$  superconducting films failed to show the jump in the exponent  $a$  of current-voltage characteristics,  $V \propto I^a$ , a signature of the BKT transition [7]. The discussion persists up to this day [8, 9].

The precondition for the BKT transition, the logarithmic intervortex interaction, is satisfied only at distances short relative to  $\Lambda = 2\lambda^2/d$  ( $\lambda$  is the London penetration depth of the bulk material and  $d$  is the film thickness). For this reason, the search for the transition has been conducted in samples of the size  $L < \Lambda$ . It is argued here that even in small samples the interaction is not logarithmic: due to the boundary conditions at the film edges the interaction turns into a short-range near exponential decay. The main conclusion therefore is that the BKT transition could not happen in thin superconducting films of any size on insulating substrates (unlike in layered compounds where the interaction between pancake vortices is logarithmic [10]). If however the film is placed on a superconducting substrate and separated from it by an insulating layer of the thickness  $s$ , the logarithmic interaction on all distances greater than  $s$  is recovered and the BKT transition should take place.

The situation is different for ac response of thin films. The characteristic separation of vortices  $l_\omega \propto 1/\omega$  contributing to the 2D response might be small at large frequencies  $\omega$  and therefore can be recorded even in small samples, see Ref. 11 and references therein. We do not consider ac phenomena here.

*Approach.* We begin with a brief review of an approach

to vortices in thin films suggested in Ref. [12]; although not common this approach allows one to evaluate energies in a direct manner, the advantage relevant for our purpose. As was stressed by Pearl [13], a large contribution to the vortex energy in thin films comes from stray fields. In fact, the problem of a vortex in a thin film is reduced to that of the field distribution in free space subject to certain boundary conditions at the film surface. Since  $\text{curl } \mathbf{h} = \text{div } \mathbf{h} = 0$  out the film, one can introduce a *scalar* potential for the *outside* field:

$$\mathbf{h} = \nabla \varphi, \quad \nabla^2 \varphi = 0. \quad (1)$$

To formulate the boundary conditions for the outside Laplace problem, consider a film of thickness  $d \ll \lambda$  occupying the  $xy$  plane. For a vortex at  $\mathbf{r} = 0$ , the London equations for the film interior read after averaging over the film thickness:

$$h_z + \frac{2\pi\Lambda}{c} \text{curl}_z \mathbf{g} = \phi_0 \delta(\mathbf{r}), \quad (2)$$

where  $\mathbf{g}(\mathbf{r})$  is the sheet current density,  $\mathbf{r} = (x, y)$  and  $\phi_0$  is the flux quantum.

In a thin film, the Maxwell equation  $4\pi\mathbf{j}/c = \text{curl } \mathbf{h}$  is reduced to relations between the sheet current and discontinuities of the tangential fields:

$$4\pi\mathbf{g}/c = \hat{\mathbf{z}} \times [\mathbf{h}(+0) - \mathbf{h}(-0)]. \quad (3)$$

One substitutes Eq. (3) in (2) and uses  $\text{div } \mathbf{h} = 0$  to obtain:

$$h_z - \Lambda[\partial_z h_z(+0) - \partial_z h_z(-0)]/2 = \phi_0 \delta(\mathbf{r}). \quad (4)$$

This equation expressed in terms of the potential  $\varphi$  along with conditions at infinity constitute the boundary conditions for the Laplace problem, Eq. (1), for the field distribution outside the film.

Consider the case in which the half-spaces above and under the film are vacuum (or a non-magnetic insulator). The general form of the potential that vanishes at  $z \rightarrow +\infty$  of the empty upper half-space is

$$\varphi(\mathbf{r}, z) = \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \varphi(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r} - kz}. \quad (5)$$

Here,  $\varphi(\mathbf{k})$  is the 2D Fourier transform and  $k^2 = k_x^2 + k_y^2$ . In the lower half-space one has to replace  $z \rightarrow -z$ . Due to the symmetry, the boundary condition (4) becomes  $\partial_z \varphi(+0) - \Lambda \partial_z^2 \varphi(+0) = \phi_0 \delta(\mathbf{r})$  that yields the Fourier transform of the potential in the upper half-space:

$$\varphi = -\frac{\phi_0}{k(1+k\Lambda)}. \quad (6)$$

This provides  $h_z(\mathbf{k}) = -k\varphi(\mathbf{k})$  and  $h_{x,y}(\mathbf{k}) = ik_{x,y}\varphi(\mathbf{k})$ , i.e. the fields everywhere in the free space as well as the sheet currents due to a single vortex in an *infinite* film. One can easily verify that this solution coincides with that given by Pearl [13].

*Energy.* We now establish connection between vortex energy and the potential  $\varphi$ . We begin with the general situation of a vortex in a *finite* bulk sample. The energy consists of the London energy (magnetic + kinetic) inside the sample,  $\epsilon^{(i)} = \int [h^2 + (4\pi\lambda j/c)^2] dV/8\pi$  and the magnetic energy outside,  $\epsilon^{(a)} = \int h^2 dV/8\pi$ . Then, for the potential introduced in Eq.(1) and gauged to zero at  $\infty$  (which is possible in *zero applied field*) one has  $8\pi\epsilon^{(a)} = \oint \varphi \mathbf{h} \cdot d\mathbf{S}$  where the integral is over the sample surface with  $d\mathbf{S}$  directed inward the material. The London part is transformed integrating by parts the kinetic term:  $8\pi\epsilon^{(i)} = (4\pi\lambda^2/c) \oint (\mathbf{j} \times \mathbf{h}) \cdot d\mathbf{S}$  where the integral is over the sample surface and the surface of the vortex core. The integral over the sample surface is further transformed:  $\oint d\mathbf{S} \cdot (\mathbf{j} \times \nabla \varphi) = \oint d\mathbf{S} \cdot \varphi (\nabla \times \mathbf{j})$  [14]. Combining the result with  $\epsilon^{(a)}$ , one obtains  $\oint d\mathbf{S} \cdot \varphi (\mathbf{h} + 4\pi\lambda^2 \text{curl} \mathbf{j}/c)$  where the expression in parenthesis is  $\phi_0 \hat{\mathbf{v}} \delta^{(2)}(\mathbf{r} - \mathbf{r}_v)$  where  $\hat{\mathbf{v}}$  is the direction of the vortex crossing the surface at the point  $\mathbf{r}_v$ , and  $\delta^{(2)}(\mathbf{r} - \mathbf{r}_v)$  is the 2D  $\delta$  function. One then obtains:

$$\epsilon = \frac{\phi_0}{8\pi} [\varphi(\mathbf{r}_{ent}) - \varphi(\mathbf{r}_{ex})] - \frac{\lambda^2}{2c} \oint_{core} d\mathbf{S} \cdot (\mathbf{h} \times \mathbf{j}); \quad (7)$$

$\mathbf{r}_{ent}$  and  $\mathbf{r}_{ex}$  are the positions of the vortex entry and exit at the sample surface (the vortex is assumed to cross the sample surface at right angles; otherwise, one should multiply the potentials by cosines of corresponding angles). For more than one vortex one has to sum up expressions (7) over all vortices. If more than one superconductor is present, Eq. (7) still holds, but  $\varphi$  as a solution of Laplace equation outside superconductors will be affected by the presence of all superconductors.

For thin films, the integral over the core surface ( $\propto d$ ) can be neglected:

$$\epsilon = \frac{\phi_0}{8\pi} \sum_{\nu} D\varphi_{\nu} \quad (8)$$

where the notation  $D\varphi_{\nu} \equiv \varphi_{\nu}(\mathbf{r}_{ent}) - \varphi_{\nu}(\mathbf{r}_{ex})$  for the  $\nu$ -vortex is introduced for brevity. Due to linearity of the Laplace and London equations, one has for two vortices

$\varphi = \varphi_1 + \varphi_2$  and

$$\begin{aligned} \epsilon &= \frac{\phi_0}{8\pi} [D\varphi(1) + D\varphi(2)] \\ &= \frac{\phi_0}{8\pi} D[\varphi_1(1) + \varphi_2(1) + \varphi_2(1) + \varphi_2(2)] \end{aligned} \quad (9)$$

where the arguments 1,2 are positions of vortices. Clearly, the self-energy of the first vortex is

$$\epsilon_1^{(0)} = \frac{\phi_0}{8\pi} D\varphi_1(1) \quad (10)$$

and the interaction energy is given by

$$\epsilon_{int} = \frac{\phi_0}{8\pi} D[\varphi_2(1) + \varphi_2(1)]. \quad (11)$$

*Infinite film in vacuum.* Equations (10) and (11) are quite general and hold for films of any lateral size. In particular, for an *infinite* film in vacuum one obtains with the help of the potential (6):

$$\epsilon^{(0)} = \frac{\phi_0}{4\pi} \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \frac{\phi_0}{k(1+k\Lambda)} = \frac{\phi_0^2}{8\pi^2 \Lambda} \ln \frac{\Lambda}{\xi}, \quad (12)$$

where the cutoff at  $k_{\max} \approx 1/\xi$  is introduced to a logarithmically divergent integral. Similarly, one finds:

$$\epsilon_{int} = \frac{\phi_0^2}{8\pi \Lambda} \left[ \mathbf{H}_0\left(\frac{r}{\Lambda}\right) - Y_0\left(\frac{r}{\Lambda}\right) \right], \quad (13)$$

where  $\mathbf{H}_0$  and  $Y_0$  are Struve and Bessel functions and  $r$  is the distance between vortices. At distances  $r \gg \Lambda$  this yields  $\epsilon_{int} = \phi_0^2/4\pi^2 r$  (as for two point “magnetic charges”  $\phi_0/2\pi$ ) showing that at large distances the role of stray fields is dominant. For  $r \ll \Lambda$ , the interaction is logarithmic,

$$\epsilon_{int} = \frac{\phi_0^2}{4\pi^2 \Lambda} \ln \frac{2\Lambda}{r}, \quad (14)$$

that led to a statement that the BKT transition should be searched for in samples of the size  $L \ll \Lambda$ . We show below that this statement is incorrect.

*Small samples in vacuum.* To consider small samples, one turns back to the basic Eq. (2). The currents  $\mathbf{g}(\mathbf{r})$  can be found by solving Eq. (2) combined with the continuity equation and the Biot-Savart integral which relates the field  $h_z$  to the surface current:

$$\text{div} \mathbf{g} = 0, \quad h_z(\mathbf{r}) = \int d^2 \mathbf{r}' [\mathbf{g}(\mathbf{r}') \times \mathbf{R}/cR^3]_z; \quad (15)$$

$\mathbf{R} = \mathbf{r} - \mathbf{r}'$ . To satisfy  $\text{div} \mathbf{g} = 0$  it is convenient to deal with a scalar stream function  $G(\mathbf{r})$  such that  $\mathbf{g} = \text{curl} G \hat{\mathbf{z}}$ . Alternatively, the sheet current can be expressed in terms of the derivatives of the potential  $\varphi(\mathbf{r}, +0)$  at the upper film face:

$$g_x = c \partial_y \varphi / 2\pi, \quad g_y = c \partial_x \varphi / 2\pi. \quad (16)$$

Therefore,  $G(\mathbf{r})$  is proportional to  $\varphi(\mathbf{r}, z = +0)$ :

$$\varphi(\mathbf{r}, +0) = -2\pi G(\mathbf{r})/c \quad (17)$$

(a possible additive constant is zero since both  $\varphi$  and  $G$  are gauged to zero at  $\infty$ ). Since the energies are expressed in terms of  $\varphi$  at vortex positions, Eq. (17) shows that to evaluate vortex energies and their interaction it suffices to find the current distribution  $G(\mathbf{r})$ .

The problem of current distribution for samples of arbitrary size is difficult: the London Eq. (4) combined with Biot-Savart law (15) make an integro-differential equation for  $\mathbf{g}$ . However, for small samples,  $L \ll \Lambda$ , it is manageable because as is seen from Eq. (15) the field  $h_z \sim g/c$  whereas the term with current derivatives in Eq. (2) is of the order  $\Lambda g/cL$ . Then, Eq. (2) can be rewritten as a Poisson equation for  $G$ :

$$\nabla^2 G = -(c\phi_0/2\pi\Lambda)\delta(\mathbf{r} - \mathbf{a}). \quad (18)$$

The normal to the edge component of the current vanishes, i.e.,  $G$  is a constant along the edges which can be set zero. Thus,  $G$  is equivalent to the electrostatic potential of a linear charge  $q = c\phi_0/8\pi^2\Lambda$  situated at the vortex position  $\mathbf{a}$  and parallel to the side surface of the grounded metal cylinder with the cross-section coinciding with the thin-film sample. A rich library of the 2D electrostatics is instrumental in solving for vortex currents for a variety of film shapes with linear dimensions less than  $\Lambda$ ; see, e.g., Ref. [15] for the solution of Eq. (18) for a rectangular film.

*Thin-film strips in vacuum.* Most of experiments of our interest are done on long thin-film strips. For a strip along  $y$  with edges at  $x = 0$  and  $x = W \ll \Lambda$ , the solution of Eq. (18) for a vortex placed at  $\mathbf{a} = (a_x, a_y)$  with zero boundary conditions at the edges reads:

$$\tanh \frac{G}{2q} = \frac{\sin(\pi a_x) \sin(\pi x)}{\cosh[\pi(y - a_y)] - \cos(\pi a_x) \cos(\pi x)}, \quad (19)$$

where for brevity  $W$  is used as a unit length (see, e.g., Refs. [15]) or [16]. Due to the edges,  $G$  does not depend exclusively on  $|\mathbf{r} - \mathbf{a}|$ ; note however that  $G(\mathbf{r}, \mathbf{a}) = G(\mathbf{a}, \mathbf{r})$ . It is straightforward now to find the energies of vortices in a strip and their interaction with the help of general formulas (10), (11), and (17).

The self-energy of a vortex at the position  $x = a, y = 0$ ,  $\epsilon = \phi_0 G(a)/2c$ , is logarithmically divergent. Introducing the cutoff at  $|\mathbf{r} - \mathbf{a}| = \xi$  one obtains [12]:

$$\epsilon^{(0)}(a) = \frac{\phi_0^2}{8\pi^2\Lambda} \ln \left( \frac{2W}{\pi\xi} \sin \frac{\pi a}{W} \right). \quad (20)$$

The interaction (11) of two vortices at  $\mathbf{a}_1$  and  $\mathbf{a}_2$  is

$$\epsilon_{int} = \frac{\phi_0^2}{8\pi^2\Lambda} \ln \frac{\cosh[\pi(y_1 - y_2)] - \cos[\pi(x_1 + x_2)]}{\cosh[\pi(y_1 - y_2)] - \cos[\pi(x_1 - x_2)]} \quad (21)$$

where the coordinates are given again in units of  $W$ . (Formally similar interaction exists between Abrikosov vortices parallel to the thin film [17].) Hence the interaction is not proportional to the logarithm of the intervortex distance as required by BKT (except at distances of the order  $\xi$  where the present theory breaks down). E.g., for  $y_1 = y_2$  we have (in conventional units):

$$\epsilon_{int} = \frac{\phi_0^2}{4\pi^2\Lambda} \ln \left| \frac{\sin[\pi(x_1 + x_2)/2W]}{\sin[\pi(x_1 - x_2)/2W]} \right|. \quad (22)$$

For vortices in the strip middle ( $x_1 = x_2 = W/2$ ) separated by  $y$ ,

$$\epsilon_{int} \approx \frac{\phi_0^2}{4\pi^2\Lambda} \ln \left| \coth \left( \frac{\pi y}{2W} \right) \right|. \quad (23)$$

This gives for  $y > W$ :

$$\epsilon_{int} = \frac{\phi_0^2}{2\pi^2\Lambda} \exp \left( -\frac{2\pi y}{W} \right). \quad (24)$$

Thus, for separations larger than  $W/2\pi$ , the intervortex interaction is in fact exponentially weak and short-range. Physically, this happens because the second vortex feels not only the “bare” first, but also the infinite chain of  $\pm$  images which one has to introduce to satisfy the boundary conditions at the edges. The possibility of BKT transition in thin-film bridges of YBCO similar to those studied in [6] has been examined experimentally [4] and theoretically [5] (see references therein) with no positive outcome. Given the above argument, one can say that the short range interaction in small samples is the reason for this failure.

*Superconducting substrate.* Up to this point, we have discussed a “free standing” film or, better to say, a thin superconducting film placed on an insulating non-magnetic substrate so that the symmetry of the upper and lower half-spaces could be utilised. The situation changes if the film is placed on a superconducting substrate being separated from it by an insulating layer to prevent the Josephson coupling to the substrate. The vortex magnetic flux  $\phi_0$  is channeled into the space between the film and the screening substrate so that the radial field component along with azimuthal sheet currents vary as  $1/r$  at large distances. This results in the Lorentz interaction force of two vortices varying as  $1/r$  and, therefore, in the logarithmic interaction energy.

To confirm this quantitatively, consider a film situated at a  $z = s$  above a superconducting substrate occupying the half-space  $z < 0$ . If  $s$  is large enough to suppress the Josephson interaction, the problem is reduced to solving the Laplace equation (1) for the potential  $\varphi_A(\mathbf{r}, z)$  in the free space  $z > s$  (the domain A) and for  $\varphi_B(\mathbf{r}, z)$  in the domain B between the film and the substrate,  $0 < z < s$ . A simple method of doing this is described in Ref. 18. One looks for  $\varphi_A(\mathbf{r}, z)$  in the form (5) with the 2D Fourier

transform  $\varphi_A(\mathbf{k}) e^{-kz}$ . Similarly, in the finite domain B,  $\varphi_B(\mathbf{k}, z) = C_1(\mathbf{k}) e^{kz} + C_2(\mathbf{k}) e^{-kz}$ . The boundary conditions at  $z = s$  are given by the field continuity and by the London equation (2). One further simplifies the problem of the substrate screening by setting the substrate penetration depth to zero, i.e.,  $h_z(z = 0) = 0$  at the substrate surface; this gives  $C_1 = C_2 \equiv C$ . After simple algebra one obtains:

$$\varphi_A = -2C e^{ks} \sinh ks = -\frac{\phi_0 e^{ks} \sinh ks}{k(\sinh ks + k\Lambda e^{ks}/2)}. \quad (25)$$

Given the potentials above and under the film, one uses Eq. (10) to calculate the vortex energy:

$$\epsilon = \frac{\phi_0^2}{16\pi^2} \int \frac{dk e^{ks}}{\sinh ks + k\Lambda e^{ks}/2}, \quad (26)$$

The lower limit of integration is the inverse sample size  $1/L$ , whereas the upper one is  $1/\xi$ . One can estimate this integral splitting the integration domain in two:  $s/\Lambda < ks < 1$  and  $1 < ks < s/\xi$ . The contributions to the integral are estimated as  $(2/\Lambda) \ln(L/s)$  and  $(4/\Lambda) \ln(s/\xi)$ . This gives

$$\epsilon \approx \frac{\phi_0}{4\pi^2\Lambda} \ln \frac{\sqrt{Ls}}{\xi}. \quad (27)$$

The interaction energy is found with the help of the general result (11):

$$\epsilon_{int} = \frac{\phi_0^2}{8\pi^2} \int_{1/L}^{1/\xi} dk J_0(kr) \frac{\cosh ks + e^{ks} \sinh ks}{\sinh ks + k\Lambda e^{ks}/2}. \quad (28)$$

The oscillating Bessel function truncates the integral at  $k \approx 1/r$ , so that in the relevant part of the integration domain  $ks < s/r \ll 1$  for intervortex distances exceeding  $s$ . One readily estimates:

$$\epsilon_{int} \approx \frac{\phi_0^2}{4\pi^2\Lambda} \ln \frac{\Lambda}{r}, \quad r > s. \quad (29)$$

Thus, the superconducting film situated parallel to the surface of a bulk superconductor should exhibit the BKT transition, unlike the case of insulating substrate, a verifiable conclusion.

To summarize, it is shown that in small thin-film samples on insulating substrates, edge effects modify the vortex-vortex interaction making it short-range, unlike the logarithmic long-range interaction needed for the BKT transition. In large free-standing films this transition cannot happen because of the  $1/r$  interaction via the stray fields. This makes the BKT transition impossible in thin films of any size if they are supported by a

non-superconducting substrate. On the contrary, if the substrate is superconducting and separated from the film by an insulated layer of a thickness  $s$ , the interaction is logarithmic at all distances  $r > s$  and the BKT transition should be observable in a dc type of experiment; e.g., the dc power-law current-voltage characteristics should show the well-known jump of the power exponent at the BKT transition.

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